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Virtual-site correlation mean field approach to criticality in spin systems

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ABSTRACT

We propose a virtual-site correlation mean field theory for dealing with interacting many-body systems. It involves a coarse-graining technique that terminates a step before the mean field theory: While mean field theory deals with only single-body physical parameters, the virtual-site correlation mean field theory deals with single- as well as two-body ones, and involves a virtual site for every interaction term in the Hamiltonian. We generalize the theory to a cluster virtual-site correlation mean field, that works with a fundamental unit of the lattice of the many-body system. We apply these methods to interacting Ising spin systems in several lattice geometries and dimensions, and show that the predictions of the onset of criticality of these models are generally much better in the proposed theories as compared to the corresponding ones in mean field theories.

1. Introduction and main results

It is rarely possible to treat an interacting many-body system exactly, and hence it is important to obtain approximate methods to deal with them. The mean field theory (MFT) [1–5], introduced by Weiss in 1907, is a very useful tool available to many-body physics to investigate properties of interacting many-body systems. There are several versions of MFT available, and a typical one reduces the interacting many-body system to a one-body system, while still retaining footprints of the many-body parent as an undetermined parameter, which is to be determined by a certain self-consistency relation (MF equation).

We propose that parallel to, but clearly different from, the mean field class of theories [1–5], there exists a virtual-site correlation mean field class of theories to treat interacting many-body systems, that deals with one-body and two-body physical parameters in its self-consistency equations. The theory reduces the many-body classical system into a two-body one. In contrast to MFT, in virtual-site correlation mean field theory (VMFT), the undetermined parameter(s) depends on a two-site physical quantity (like, two-point correlation), possibly along with a single-site quantity, of the many-body parent. This parameter is then determined by the self-consistency relations (VMFT equations) equating, e.g. the two-point correlation of the many-body parent with that of the VMFT-reduced two-body system. The main motivation for such consideration is based on the fact that two-point correlation functions play an important role in detecting cooperative physical phenomena in many-body systems [6,7], and therefore contain more information about a physical system than the single-site properties like magnetization. Correspondingly, a mean-field-like theory that *begins* with two-site properties like correlations at the level of the self-consistency equations can potentially be more effective than those that begin with single-site ones.

The mean field class of theories can be thought of as an ultimate form of coarse-graining of the many-body system, in that it reduces the interacting many-body Hamiltonian to single-body terms, and deals with single-body physical parameters in its self-consistency equations [1–5]. The virtual-site correlation mean field class of theories proposes to stop a step before in the coarse-graining process, and reduces the parent Hamiltonian to a finite number of two-body terms, and deals with single- as well as two-body terms in its self-consistency equations.

An interesting generalization of the mean field approach to many-body systems is the cluster mean field theory (CMFT) [8–10], where one reduces the many-body system to a fundamental unit ("cluster") of the many-body lattice. Again, the undetermined parameter, generated by the transition of the parent Hamiltonian into the CMFT Hamiltonian, is a one-site physical quantity (like, magnetization) of the many-body parent, and it is determined by the self-consistency relation (CMF equation) equating the parameter to the same one-site quantity obtained from the cluster. We stress here that the self-consistency relations in the standard MFT and CMFT are obtained by equating magnetization-like one-site physical quantities, and hence are different from the virtual-site correlation mean field theory. The differences, both operational and result-wise, between VMFT and CMFT will be further underlined later (in particular, in Table 1).

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Table 1
A comparison of the critical temperatures obtained for the nearest-neighbor Ising model in different lattices and geometries. The numbers in the table are in units of $k_B T/J$. "NA" = "Not applicable". The last column marked "Exact" displays either exact or series results.

Lattice	MF	VMF	CMF	CVMF	Exact
Linear	2	1	1.28	NA	0
Hexagonal	3	2	2.335	1.61	1.52
Square	4	3	3.5	2.43	2.27
Triangular	6	5	5.64	4.16	3.64
Cubic	6	5	5.49	3.62	4.51

In the present work, along with applying a VMFT approach to deal with critical phenomena in interacting systems, we also extend the VMFT to a "cluster VMFT" (CVMFT) that reduces the many-body system to a fundamental unit of the many-body lattice. In contrast to CMFT, in CVMFT, the undetermined parameters depend *both* on one-site and two-site physical quantities (e.g., on magnetization and two-site correlation) of the many-body parent. These parameters are then determined via *coupled* self-consistency equations (CVMFT equations) equating e.g. the magnetization of the original many-body system with that of the (CVMFT-reduced) cluster, and the two-point correlation of the many-body parent with that of the cluster.

We apply the VMF and CVMF theories to the nearest-neighbor Ising model in one, two (hexagonal, square, and triangular), and three (cubic) dimensional lattices. The results are given in Table 1. In all the cases considered, in the different dimensions and geometries, VMFT gives better predictions over MFT, and CVMFT gives better predictions over CMFT.

Several other interesting generalizations of the mean field theory exist in the literature, including the Bethe–Peierls–Weiss approximation [11–15], the Onsager reaction field theory [16–18], the diagrammatic expansion method [19–21], the self-consistent correlated field theory [22], the screened magnetic field theory [23], and the correlated cluster mean field theory [24], to mention a few (see also [25]). Extensions of the virtual-site correlation mean field theory in these directions are also possible, and will be pursued later. Meanwhile, let us note here that all the above important examples, in the MF class of theories, deal with single-body physical parameters in the respective self-consistency equations. In contrast, the VMF class of theories deal with single- as well as two-body physical parameters in the VMFT class self-consistency equations.

Along with the interesting generalizations of the mean field theory mentioned above, there also exists the cluster variation method [26–32], where the free energy of an interacting system is approximated as a sum of internal energy and entropy, running over a set of clusters, and only those terms are retained in the cumulant expansion of the entropy which correspond to the set of clusters. We also note here about the dynamical cluster approximation method and the cellular dynamical mean field theory, which are extensions of the mean field theory, where self-consistency conditions employ certain non-local Green functions [33–35]. The dynamical cluster approximation method [33,34] is an extension of the dynamical mean field theory [36,37] that includes short-range correlations in addition to the considerations in the dynamical mean field theory, by an iterative self-consistency scheme taking the single-site dynamical mean field approximation to a cluster. The cellular dynamical mean field theory [35] is another generalization of the dynamical mean field approximation from the single-site scenario to that of the cluster, by incorporating ideas similar to those that led to the dynamical mean field theory from the coherent potential approximation [38–42], but for interacting systems. As we will see below, VMFT deals with a two-body Hamiltonian irrespective of the lattice geometry. See also [43,44]. In particular, in the Tóth–Lent method of Ref. [43], the parent Hamiltonian is reduced to a two-body one, while self-consistency equations are composed in terms of single-site parameters. On the other hand, in Ref. [44], the parent Hamiltonian is reduced to a two-body one, and the self-consistency equation is written in terms of two-site as well as single-site parameters. In this Letter, we modify the method in Ref. [44] so that it is fit for applications in further domains, and also generalize it to a cluster method.

2. Virtual-site correlation mean field

Before presenting the virtual-site correlation mean field approach to spin models, let us briefly describe the mean field theory for such systems. Consider the nearest-neighbor Ising model

$$H = -J \sum_{\langle \vec{i}\,\vec{j}\rangle} \sigma_{\vec{i}} \sigma_{\vec{j}} - h \sum_{\vec{i}} \sigma_{\vec{i}}, \tag{1}$$

which represents a system of interacting spin-1/2 particles (Ising spins) on a d-dimensional lattice of an arbitrary fixed geometry. The coupling strength J and the field h are positive, and $\sigma_{\vec{i}} = \pm 1$ represents the value of the Ising spin at the site $\vec{i}$. $\langle \vec{i}\,\vec{j}\rangle$ indicates that the corresponding sum runs over nearest-neighbor lattice sites only.

The mean field theory consists in assuming that a particular spin, say at $\vec{i}_0$, is special, and replacing all other spin operators by their mean values. Denoting the mean values of the spin operator $\sigma_{\vec{i}}$ at the site $\vec{i}$ by m (average magnetization), leads to an MFT Hamiltonian [1–5], which we denote as H_{MFT}. One then solves the self-consistency equations (mean field equations)

$$m = \sum_{\mathcal{CF}(\mathcal{I})} \sigma \rho_{MFT}^{\beta}, \tag{2}$$

for m. Here ρ_{MFT}^{β} is the mean field canonical equilibrium state $\exp(-\beta H_{MFT})/Z_{MFT}$, $Z_{MFT} = \sum_{\mathcal{CF}(\mathcal{I})} \exp(-\beta H_{MFT})$ is the MF partition function, $\beta = \frac{1}{k_B T}$, with T denoting temperature on the absolute scale, and k_B the Boltzmann constant. Here, and in the rest of the Letter, $\mathcal{CF}(\mathcal{I})$ will denote all Ising configurations of all the spins involved in that particular case. In the MF equation as well as in the MF partition function, there is just a single spin left, and $\mathcal{CF}(\mathcal{I})$ denotes the set of the two possibilities thereof. Substituting m in H_{MFT} and ρ_{MFT}^{β}, one can find the single-body physical properties of the system in the mean field limit.

The virtual-site correlation mean field theory begins by noting that the square of an Ising spin random variable is unity. The two-body interaction Hamiltonian that we are dealing with, can be thought of as an N-body interaction Hamiltonian (N being the total number of Ising spins in the system), in each term of which, all but two random variables are constant (= unity). Let us call it a unit random variable. Since the square of any Ising random variable is unity, we can replace a unit random variable on a site that is neighboring the nontrivial interacting spins of an interaction term, by the square the Ising random variable at that site, for all the interaction terms in the Hamiltonian. For definiteness, let us consider a (two-dimensional) square lattice. Therefore, the interaction term

$$\sigma_{k-1,l}\sigma_{k,l} \tag{3}$$

in a Hamiltonian on a square lattice can be replaced by

$$\sigma_{k-1,l}\sigma_{k,l}\sigma_{k+1,l}\sigma_{k+1,l}. \tag{4}$$

We would like to mention here that the theory proposed in [44] uses an apparently similar method. VMFT is applied by using the fact that $\sigma_{k-1,l}\sigma_{k,l}\sigma_{k+1,l}\sigma_{k+1,l} = \sigma_{k-1,l}\sigma_{k,l}$ holds for the classical